Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H15ClF8O5/c1-29-11-7-9(18)5-6-10(11)31-13(28)4-2-3-12(27)30-8-15(21,2

InchiKey: BIPFNQRGCGDMAC-UHFFFAOYSA-N

Formula: C17H15ClF8O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 486.74

Physical Properties

Property code	Value	Unit	Source
gf	-1951.76	kJ/mol	Joback Method
hf	-2418.59	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.138		Crippen Method
mcvol	273.780	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	821.46	K	Joback Method
tc	1010.62	K	Joback Method
tf	526.26	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.89	J/mol×K	821.46	Joback Method
cpg	834.05	J/mol×K	852.99	Joback Method
cpg	844.32	J/mol×K	884.51	Joback Method
cpg	853.75	J/mol×K	916.04	Joback Method
cpg	862.38	J/mol×K	947.57	Joback Method
cpg	870.25	J/mol×K	979.10	Joback Method
cpg	877.43	J/mol×K	1010.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume